

About you and your group

1. Please provide your name and institution.

Name

Institution

Country

2. What is your role?

- Professor
- Group leader
- Post-doc
- Other

Other (please specify)

3. How many members does your group have currently?

Senior Staff

Postdocs

Graduate Students

4. Considering the involvement with theory and modeling, how many people in your group fall into the respective categories? For people involved in more than one activity, just count them into each relevant category.

Code authors

Modeling users

Consumers of model results

Methods and applications

5. What types of modeling method do you and your group develop?

- Higher level theory
- Density functional theory
- Semi-empirical methods including DFTB
- Classical simulation
- Other

Please specify Other

6. What types of 'observables' and properties do you determine? Observables and properties refer to the quantities that are calculated directly from the simulation.

Frequently	<input type="text"/>
Occasionally	<input type="text"/>
Rarely	<input type="text"/>

7. What fields of application does your group work on in general? These include types of materials and target applications of materials, e.g. alloy, semiconductors, displays etc.

Frequently	<input type="text"/>
Occasionally	<input type="text"/>
Rarely	<input type="text"/>

Industry Collaborations

8. What modeling methods do you and your group use in industry collaborations?

	Frequently	Occasionally	Never
Higher level theory	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Density functional theory	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Semi-empirical methods including DFTB	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Classical simulation	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Other	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>

Please specify Other

9. Considering industry collaborations, what types of applications is your group involved in?

Frequently	<input type="text"/>
Occasionally	<input type="text"/>
Rarely	<input type="text"/>

10. What industry sectors do the companies you work with represent?

- Basic chemicals
- Specialty chemicals
- Materials
- Electronics
- Automotive and aerospace
- Pharmaceuticals
- Consumer Packaged Goods
- Software
- Other

Please specify Other

11. How frequently have you been engaged in the following industry interactions in the last 3 years?

	0 times	1-2 times	3-6 times	7-11 times	>= 12 times
Informal personal interactions (i.e. not involving a signed agreement)	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Consultancy and contract research (formal, with specific objectives)	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Research funded by industry (typically collaborative research projects)	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Training company employees	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Setting up a physical facility for industry or a spin-off company	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Other	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>

Please specify Other

12. In the last 3 years, how many different companies have you and your team worked with (i.e. had some sort of funding from)?

In government funded projects

Without government funding

13. In the last 3 years, how many different industry funded projects of what different duration has your team been involved with? (Count different projects with the same company separately).

	With government funding	Without government funding
up to 3 weeks long	<input type="text"/>	<input type="text"/>
3 weeks to 3 months long	<input type="text"/>	<input type="text"/>
3 months to 1 year long	<input type="text"/>	<input type="text"/>
Longer than 1 year	<input type="text"/>	<input type="text"/>

14. What is the job function of your main contact in these industry projects?

	In most cases	Sometimes	Rarely	Never
R&D manager	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Lab scientist (e.g. characterization)	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Computational scientist	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Engineer (chemical/material/electronics)	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Other	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>

Please specify Other:

Measures of success

15. What is your longest standing industry collaboration?

Duration in months:

Comment:

16. How many renewals/projects have you had with the same company?

Number of projects:

17. How many companies do you collaborate with on average at a given time?

18. What percentage of these companies are in Europe?

19. What are the main reasons for your industry collaborators to enter into projects?

- Expertise of academic PI.
- To gain access to new ideas and insights.
- To access particular skills that are not available in house.
- To access particular techniques that are not available in-house.
- To overcoming bottlenecks in existing R&D projects.
- To assess potential of new directions not currently pursued in-house.
- To substitute some of their R&D.
- To reduce R&D costs.
- Open Innovation objectives.
- Other

Please specify Other expectations

20. What measures of success are applied by companies?

- Patent applications
- New insights into cutting-edge science/technology
- Breakthroughs in R&D projects
- Speeding up R&D project
- Cost saving: reduction/steering of experimentation
- Other ROI measures (please specify)

Please specify Other Return on Investment (ROI) measure

21. What have been the key success outcomes from your perspective? Please comment and provide numbers where relevant.

Publications	<input type="text"/>
Patent applications	<input type="text"/>
Royalties	<input type="text"/>
New methods developed	<input type="text"/>
Students trained	<input type="text"/>
Funding for research	<input type="text"/>
Effect on research assessments	<input type="text"/>
Other (please comment)	<input type="text"/>

22. How many students have been trained in your group in the last 5 years that then went on to work in industrial R&D?

Entered into computational roles	<input type="text"/>
Other roles in industrial R&D	<input type="text"/>

23. Please provide examples and success stories.

Many thanks for taking part in this survey!